

Quantum phase transition in easy-axis antiferromagnetic Heisenberg spin-1 chain

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Abstract

The fidelity and entropy in an easy-axis antiferromagnetic Heisenberg spin-1 chain are studied numerically. By using the method of density-matrix renormalization-group, the effects of anisotropy on fidelity and entanglement entropy are investigated. Their relations with quantum phase transition are analyzed. It is found that the quantum phase transition from Haldane spin liquid to Néel spin solid can be well characterized by the fidelity. The phase transition can be hardly detected by the entropy. But it can be successfully detected by the first deviation of the entropy.

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I. INTRODUCTION

In condense matter physics, quantum phase transitions imply fluctuations, which happened at the zero temperature [1]. When a controlling parameter changes across critical point, some properties of the many-body system will change dramatically. Many results show that entanglement existed naturally in the spin chain when the temperature is at zero. The quantum entanglement of a many-body system has been paid much attention since the entanglement is considered as the heart in quantum information and computation [2, 3]. As the bipartite entanglement measurement in a pure state, the von Neumann entropy [4] in the antiferromagnetic anisotropic spin chain [5] and isotropic spin chain [6] are investigated respectively. By using the cross fields of quantum many-body theory and quantum-information theory, von Neumann entropy is applied to detect quantum critical behaviors [7–11]. A typical example is that Osborne solved exactly one-dimensional infinite-lattice transverse-field Ising model to obtain entropy by the Jordan-Wigner transform. The entropy predicts the quantum phase transition successfully [8]. Moreover, another concept from quantum information science, the ground state fidelity has been used to qualify quantum phase transitions in the last few years [12–24]. Because the fidelity is a measure of similarity between states, the fidelity should drop abruptly at critical points as a consequence of the dramatic changes in the structure of the ground states, regardless of what type of internal order is present in quantum many-body states. This result is the orthogonality of different ground states due to state distinguishability. Many results shown that the fidelity and the entanglement entropy have similar predictive power for identifying quantum phase transitions in the most systems [23, 24]. However, the ground state fidelity is a model-dependent indicator for quantum phase transitions. It cannot be used to characterize the Berezinskii-Kosterlitz-Thouless (BKT) transition [25, 26]. The BKT-like transition occurs at Heisenberg isotropic spin chain with next-nearest-neighbor and in antiferromagnetic anisotropic Heisenberg model with $\Delta = 1$ [25]. Entanglement, fidelity and their relations with quantum phase transition in high spin chain, just like spin-1 chain need to be further investigated.

In this paper, the fidelity and entanglement in the easy-axis spin-1 chain are numerically investigated by using the density-matrix renormalization-group (DMRG) technique. In section II, the Hamiltonian of easy-axis spin-1 chain and its critical property are presented. In section III, the effects of anisotropic interaction on fidelity is investigated and its relation with quantum phase

transition is analyzed. The effects of anisotropic interaction on entanglement entropy is calculated and its relation with quantum phase transition is analyzed in section IV. At last, a discussion concludes the paper.

II. HAMILTONIAN AND ITS CRITICAL PROPERTY

It is known that there is a gap in the spectrum of isotropic Heisenberg spin-1 chain in the thermodynamic limit. The gap between the ground state and the first excited state energy is usually called Haldane gap [27]. The Hamiltonian of an anisotropic Heisenberg antiferromagnetic spin-1 chain of N sites can be given by

$$H = J \sum_{i=1}^{N-1} (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z), \quad (1)$$

where $S_i^\alpha (\alpha = x, y, z)$ are spin operators on the i -th site and N is the length of the spin chain. The parameter $J > 0$ denotes the antiferromagnetic coupling and $J = 1$ is considered in the paper. The parameter Δ is anisotropic interaction, $0 < \Delta < 1$ is the easy-plane anisotropy and $\Delta > 1$ is the easy-axis anisotropy. It is predicted that a novel phase $\Delta_{C1} \in [0 \sim 0.2] < \Delta < \Delta_{C2} = 1.17$ appears between the XY phase and the Néel phase [28–30]. Many results suggested that a BKT transition occurs at Δ_{C1} , while that the transition at Δ_{C2} belongs to the 2D Ising universality class [31–34]. Since the fidelity cannot detect a BKT-like phase transition [25, 26], we only concentrate on quantum phase transition which happens at easy-axis anisotropy. It is found that the Hamiltonian in Eq. (1) can be transformed conveniently to give

$$H = J \sum_{i=1}^{N-1} [p(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) + S_i^z S_{i+1}^z], \quad (2)$$

where $p = 1/\Delta$. The critical point of transition from Haldane spin liquid to Néel spin solid is around $p_c \simeq 0.85$. It is noted that the model of Eq. (2) is invariant for $p \rightarrow -p$, so that the results in the paper can be equally applied to a system with a ferromagnetic coupling on the xy plane.

III. FIDELITY SUSCEPTIBILITY

The ground state fidelity can be applied to detect the existence of the quantum phase transitions. A general Hamiltonian of quantum many-body system can be written as $H(\lambda) = H_0 + \lambda H_I$ where

H_I is the driving Hamiltonian and λ denotes its strength. If $\rho(\lambda)$ represents a state of the system, the ground state fidelity between $\rho(\lambda)$ and $\rho(\lambda + \delta)$ can be defined as

$$F(\lambda, \delta) = \text{Tr}[\sqrt{\rho^{1/2}(\lambda)\rho(\lambda + \delta)\rho^{1/2}(\lambda)}]. \quad (3)$$

If the state can be written as $\rho = |\psi\rangle\langle\psi|$, the Eq. (3) can be rewritten as $F(\lambda, \delta) = |\langle\psi(\lambda)|\psi(\lambda+\delta)\rangle|$. Because $F(\lambda, \delta)$ reaches its maximum value $F_{max} = 1$ for $\delta = 0$, on expanding the fidelity in powers of δ , the first derivative $\frac{\partial F(\lambda, \delta=0)}{\partial \lambda} = 0$. By using the property, the fidelity can be written by

$$F(\lambda, \delta) \simeq 1 + \frac{\partial^2 F(\lambda, \delta)}{2\partial \lambda^2}|_{\lambda=\lambda'}\delta^2. \quad (4)$$

Therefore, the average fidelity susceptibility $S(\lambda, \delta)$ can be given by [18, 19]

$$S(\lambda, \delta) = \lim_{\delta \rightarrow 0} \frac{2[1 - F(\lambda, \delta)]}{N\delta^2}. \quad (5)$$

It is well known that it is hard to calculate the ground state fidelity because of the lack of knowledge of the ground state function. For models that are not exactly solvable, most of researchers resort to exact diagonalization to obtain the ground state for small size. This method cannot precisely quantify the quantum phase transition because the size of the system is too small. Recently, the method of density-matrix renormalization-group (DMRG) [35, 36] can be applied to obtain the ground state of the model. Moreover, the technique of calculating the overlap of two different ground states by DMRG has been used [37, 38]. For high precision, the method in [39] is used to calculate the ground state fidelity susceptibility. We calculate N up to 80 when $\delta = 0.001$ [23]. The total number of density matrix eigenstates held in system block is $m = 70$ in the basis truncation procedure. The Matlab codes of finite size density-matrix renormalization-group have double precision. They are performed with three sweep in private computer, and the truncation error is smaller than 10^{-10} .

The ground state fidelity susceptibility S is plotted as a function of anisotropic parameter p for different sizes in Fig. 1 *in dimensionless units*. It is shown that there is a peak in S . The peak of S increases when the size increases. The location of the peak decreases slightly to small value of p as N increases. The ground state fidelity F is plotted as a function of p for different sizes in the inset of Fig. 1 *in dimensionless units*. It is seen that there is a sharp valley corresponding to the peak of S . The critical point of fidelity susceptibility S and fidelity F is about $p_c = 0.85$. As we known, the fidelity measures the similarity between two states, while quantum phase transitions are

intuitively accompanied by an abrupt change in the structure of the ground state wave-function. This primary observation motivates researchers to use fidelity to predict quantum phase transitions. Up to now, the ground state fidelity and fidelity susceptibility have been applied in various many-body systems to detect quantum phase transitions successfully [12–24]. It confirms further that the Haldane spin liquid–Néel spin solid transition occurs at the point in our system.

IV. ENTANGLEMENT ENTROPY

For comparison, the ground state entanglement entropy is also used to detect the quantum phase transition. For density matrix ρ of any pure state, the entanglement entropy E_{AB} between subsystem A and B can be defined as

$$E_{AB} = -\text{Tr}(\rho_A \log_2 \rho_A) = -\text{Tr}(\rho_B \log_2 \rho_B), \quad (6)$$

where $\rho_{A(B)}$ is the reduced density matrix obtained from ρ by taking the partial trace over the state space of subsystem $B(A)$.

In order to avoid boundary effects, the entanglement entropy of two neighboring central sites of large system needs to be calculated by using the method of DMRG. The entropy of two neighboring central sites labeled $E_{N/2, N/2+1}$ is plotted as a function of anisotropy p with sizes of $N = 40, 60, 80$ in Fig. 2 *in dimensionless units*. The entanglement entropy of the two neighboring central sites increases monotonously when the anisotropy p increases. It is known that the peak or discontinuity in entanglement entropy indicates the quantum phase transition. The peak does not occur at the quantum critical point. It seems that this is due to the monogamy property [9]. We also calculate the entanglement entropy between the right-hand $N/2$ contiguous qubits and the left-hand $N/2$ contiguous qubits. The result is similar with that shown in Fig. 2. For avoiding repetition, the result is not plotted again. This means that the entropy cannot be used to predict quantum phase transition here. However, the critical properties can be captured by the derivatives of the entropy as a function of the anisotropy p [9, 40, 41].

It is noted that the transition from Haldane spin liquid to Néel spin solid is continuous and belongs to a second order quantum phase transition. It has been shown that the density matrix may be continuous but its first-order derivative is singular at a second order quantum phase transition point [42]. Consequently, we calculate the first-order derivative of entropy $dE_{N/2, N/2+1}/dp$ at the

ground state with $\delta = 0.001$. The first derivative of the central two sites entanglement entropy $dE_{N/2, N/2+1}/dp$ is plotted as a function of anisotropy p for different sizes in Fig. 3. It is seen that there is a peak in $dE_{N/2, N/2+1}/dp$. The location of the peak in $dE_{N/2, N/2+1}/dp$ moves slightly to small value of p as N increases. The critical value is about $p_c = 0.85$. It represents indeed the quantum phase transition from Haldane spin liquid to Néel spin solid.

V. DISCUSSION

In the paper, the fidelity susceptibility and entropy in an easy-axis antiferromagnetic Heisenberg spin-1 chain are studied. By using the density-matrix renormalization-group for the model, the effect of anisotropic interaction on fidelity susceptibility and entropy of large size is presented. Their relations with quantum phase transition are investigated. It is shown that the quantum phase transition from Haldane spin liquid to Néel spin solid is clearly marked by the peak (or valley) of the fidelity susceptibility (or fidelity). However, the entanglement entropy cannot have similar predictive power for revealing quantum phase transition in the system due to the monogamy property, while the first-order derivation of entropy can be used to successfully detect the quantum phase transition.

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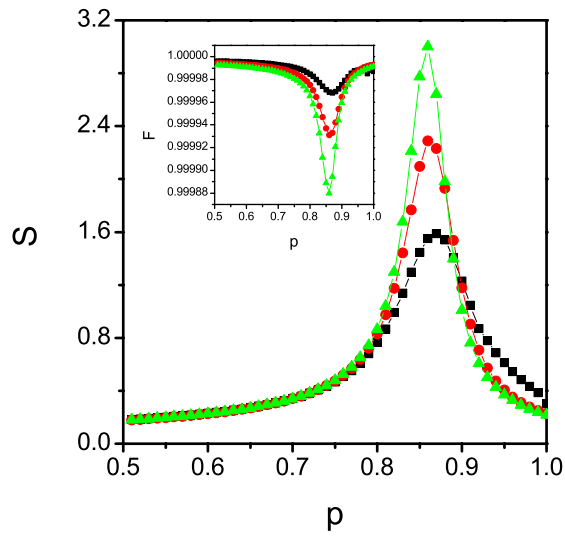


FIG. 1: The fidelity susceptibility S of the ground state is plotted as a function of anisotropy p for different size N . The fidelity F is plotted in the inset. The symbols are for $N = 40$ (\blacksquare), $N = 60$ (\bullet), $N = 80$ (\blacktriangle).

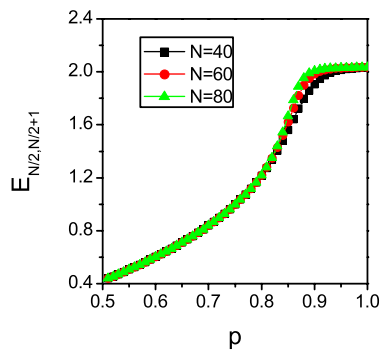


FIG. 2: The two neighboring central sites entanglement entropy $E_{N/2, N/2+1}$ is plotted as a function of anisotropy p for different size N .

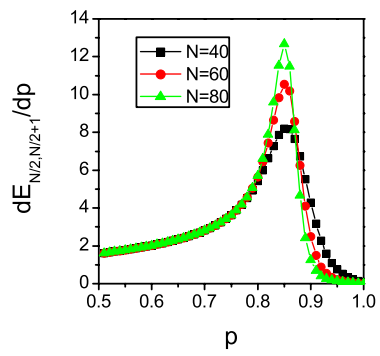


FIG. 3: The first derivative of the two neighboring central sites entanglement entropy $dE_{N/2, N/2+1}/dp$ is plotted as a function of anisotropy p for different size N .